A Multiscale Crystal Plasticity Finite Element Framework for the Representation of Slip and Deformation Twinning in HCP Metals

Hashem M. Mourad*, Curt A. Bronkhorst*, Veronica Livescu† and Irene J. Beyerlein‡

* Theoretical Divison, T-3
† Materials Science and Technology Division, MST-8
Los Alamos National Laboratory
Los Alamos, New Mexico 87545, USA
e-mail: hmourad@lanl.gov

‡ Mechanical Engineering Department
University of California, Santa Barbara
Santa Barbara, California 93106, USA

ABSTRACT

Dislocation slip and deformation twinning are the primary mechanisms by which plastic deformation takes place in metallic materials. Deformation twinning plays an especially important role in HCP metals such as titanium, where combinations of prismatic, basal and pyramidal slip may be insufficient to accommodate imposed plastic strains, particularly at low temperatures and/or under high-strain rate conditions. In addition, the reorientation of the crystallographic lattice and the introduction of twin-matrix boundaries during the twinning process affect the anisotropy of the material's response and its hardening behaviour, respectively. Recognizing the importance of twinning, researchers have made numerous efforts over the years to account for this deformation mechanism making use of homogenization schemes [1, 2]. The limitations of such approaches have motivated recent developments [2] where twins are explicitly incorporated into crystal plasticity finite element frameworks.

We present a sub-grid finite element formulation, implemented in an explicit Lagrangian framework, capable of representing the process of deformation twinning in response to dynamic loading. The proposed sub-grid formulation allows a discrete twin to be embedded within the individual finite elements that it intersects. This affords an accurate representation of the twinning process without requiring significant mesh refinement in order to resolve explicitly the lamellar morphology of a twinned region, and obviates the need for frequent remeshing to account for twin growth. A stochastic model [3] is used in this computational setting to compute the twin nucleation probability at grain boundaries, and to determine the orientation of nascent twins. Numerical results are presented and compared to experimental data and high-resolution numerical results obtained using conventional techniques, in order to illustrate the advantages of the proposed modelling and simulation strategy.

REFERENCES

[1] F. Roters, P. Eisenlohr, L. Hantcherli, D. D. Tjahjanto, T.R. Bieler, D. Raabe, "Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications," *Acta Mater.,* **58,** 1152–1211 (2010).

[2] M. Ardeljan, R. J. McCabe, I. J. Beyerlein, M. Knezevic, "Explicit incorporation of deformation twins into crystal plasticity finite element models," *Comput. Methods Appl. Mech. Engrg.*, **295**, 396–413 (2015).

[3] S. R. Niezgoda, A. K. Kanjarla, I. J. Beyerlein and C. N. Tomé, "Stochastic modeling of twin nucleation in polycrystals: An application in hexagonal close-packed metals", *Int. J. Plasticity*, **56**, 119-138 (2014).